Water dynamics on cellulose show two important populations from neutron scattering and simulations

Objective:

- To develop accurate models of hydration water in the cell wall that can inform on fundamental questions about cellulose - water interactions.

Approach:

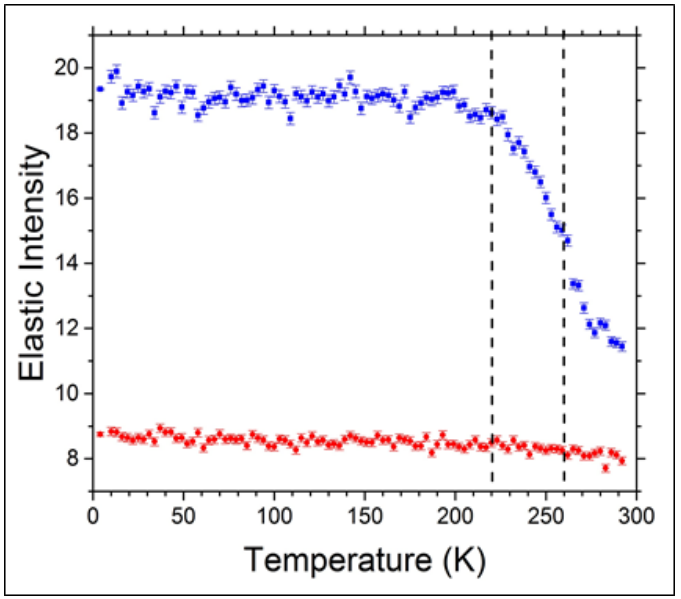
- This study presents the first systematic investigation of cellulose – water interactions using quasi-elastic neutron scattering (QENS) and molecular dynamics (MD) simulation.
- Perdeuterating cellulose (produced from *Gluconacetobacter* sp.) enabled us to directly measure the scattering of the H_2O associated with the cellulose fibers.

Results:

- The distribution of diffusion coefficients of water molecules in the simulations is bimodal, implying the existence of two populations of water molecules in the system—one tightly "bound" to the surface and the other interfibrillar and translationally mobile.

Significance:

- Understanding water's role in cellulose reactivity will help to discover the underlying processes that change biomass morphology and reactivity during different pretreatment regimes for biofuels production. The mobility of the interfibrillar water is important to enzyme and chemical attack and is distinct from the bound and bulk water.



Quasi-elastic neutron scattering (QENS) scans of dry and hydrated deuterated cellulose. Data collected at 0.9 $Å^{-1}$ are shown. The scans at other Q values showed a similar trend. The data curves with blue squares and red circles represent the hydrated and dry samples, respectively. The dashed lines denote inflection points in the curves at 220 and 260 K in the hydrated cellulose sample.

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(Dynamic Visualization of Lignocellulose Degradation …)

O'Neill, H., Pingali, S. V., Petridis, L., He, J., Mamontov, J., Hong, L., Urban, V., Evans, B., Langan, P., Smith, J. C., Davison, B. H. "Dynamics of Water Bound to Crystalline Cellulose", ***Sci. Reports*** **(2017) accepted.**

OAK RIDGE National Laboratory